Absence of the d-Density Wave State in 2D Hubbard Model

A. Macridin[1], M. Jarrell[1], and Th. Maier[2]

[1]*University of Cincinnati, Cincinnati, Ohio, 45221, USA*
[2]*Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA*
(Dated: February 2, 2008)

Using the Dynamical Cluster Approximation (DCA) we calculate the alternating circulating-current susceptibility and investigate the transition to the d-density wave (DDW) order in the two-dimensional Hubbard model. The 2×2 cluster used in the DCA calculation is the smallest that can capture d-wave order; therefore, due to the mean-field character of our calculation, we expect to overestimate d-wave transition temperatures. Despite this, we found no transition to the DDW state. In the pseudogap region the DDW susceptibility is enhanced, as predicted by the slave boson $SU(2)$ theory, but it still is much smaller than the d-wave pairing susceptibility.

Introduction The high T_c cuprates display a variety of unusual properties, which remain unexplained by conventional theories. The most intriguing physics occurs at small doping, in the proximity of antiferromagnetism and superconductivity, and is characterized by non-conventional behavior of many observables including the spin susceptibility, optical conductivity, specific heat and transport properties. Many of these unusual properties are associated with the presence of a pseudogap in the one- and two-particle spectra. Photoemission spectra show that, at small doping and above T_c, the states around the $(\pi, 0)$ point in the Brillouin Zone are gapped and Fermi segments appear around $(\pi/2, \pi/2)$, suggesting that the symmetry of the pseudogap in the hole-doped cuprates is consistent with the d-wave symmetry of the superconducting gap [1].

Based on the cuprate phenomenology, Chakravarty *et al.* [2] proposed that the pseudogap results from the competition between two ordering processes. One is d-wave superconductivity (DSC) and the other is a state characterized by long-range order of alternating orbital currents. The latter is a staggered-flux state which breaks the translational and the time-reversal symmetry and represents in fact a charge density with d-wave symmetry [3], i.e. it is a d-density wave (DDW) state. In this scenario the system evolves continuously from the DDW state to the DSC state with decreasing temperature or increasing doping, and the two states coexist up to optimal doping. The experimentally observed one-particle spectra in the pseudogap region can be well understood on the basis of the DDW state [4], which makes it a very appealing candidate for the origin of the pseudogap physics. Other properties of the cuprates, such as the resonant peak in the superconducting state and the doping dependence of superfluid density seem also to be well captured by this model [5]. Recently it was proposed the interplay of the DDW and the inter-planar tunneling of Cooper pairs to be responsible for the T_c dependence on the number of CuO_2 layers which characterizes different materials [6]. In principle, the presence of the DDW state has subtle experimental consequences, such as the formation of a magnetic moment associated with the orbital currents [7]. The interpretation of the experimental data in this respect however is still controversial.

Whereas the theory of the DDW is phenomenological, slave boson theory holds the promise of a microscopic basis which may explicitly consider static or fluctuating DDW order, as well as d-wave pairing. These are uncontrolled theories for the $t - J$ model, which is equivalent to the strong coupling limit of the Hubbard Hamiltonian. They are influenced by P.W. Anderson's *et al.* [8] idea of resonance valence bond state. The charge and the spin degrees of freedom are separated by introducing auxiliary slave bosons. The resulting mean-field theories explicitly decouple the fermion hopping along the bonds, the fermion pairing and the bosonic field, and produce phase diagrams similar to the experimental one.

We briefly discuss the main results of slave boson theories. The $t - J$ Hamiltonian has a local $SU(2)$ symmetry at half filling [9]. As a result of this symmetry the π-flux state (a staggered-flux state with the flux per plaquette equal to π) and the d-wave paring state are degenerate in the undoped model. Doping breaks the symmetry to $U(1)$ and the d-wave state becomes energetically favored [10]. The d-wave state is characterized by a finite value of the fermion pairing operator and a real superconductor emerges below the condensation temperature of the bosons. At low doping ($\delta \leq 0.05$) and for $T > 0$ the d-wave pairing becomes unstable towards the π-flux or staggered-flux state of spinons [11]. This is the standard picture of the $U(1)$ slave boson mean field theory of the $t - J$ model. However, the inclusion of other terms in the mean-field decoupling, such as the holon's flux [12], results in a existence of a DDW state at finite doping and above T_c, but exclude the coexistence of the two states.

One of the drawbacks of the $U(1)$ theory is that its solution is not stable against the fluctuations of the gauge field [13]. Fluctuations are especially important at small doping, where the energy difference between states connected via a $SU(2)$ transformation is very small (since they are degenerate at zero doping). Therefore all these states have an important contribution in the determination of the free energy.

P.A. Lee *et al.* developed a slave boson mean field

theory which is $SU(2)$ symmetric at finite doping [14]. The price paid is that one must deal with two slave bosonic fields and three constraints. The advantage of this approach is that the $SU(2)$ mean-field solution is likely superior at small doping, since it accounts better for the fluctuations between different low energy $SU(2)$ connected states. Their solution for the pseudogap region is a staggered-flux of fermions which is gauge equivalent with the d-wave pairing of fermions. However, the fermion staggered-flux state is not the same as the staggered-flux state of electrons (or the DDW state), and neither breaks time-reversal nor translation symmetry. Therefore, in $SU(2)$ theory, the pseudogap is not a broken symmetry state with long range order as it is DDW, but is rather is characterized by strong spatial and dynamic fluctuations between d-wave, s-flux and other $SU(2)$ related states.

The goal of this paper is to investigate the interplay between DDW and DSC order in the 2D Hubbard model. Using the Dynamical Cluster Approximation (DCA)[15, 16] we calculate the response functions associated with these two types of order. The DCA systematically adds non-local corrections to the Dynamical Mean Field Approximation (DMFA)[17, 18] by mapping the lattice onto a finite-size periodic cluster. The DCA mapping from the lattice to the cluster is accomplished by coarse-graining all the internal propagators in irreducible Feynman graphs in reciprocal space. Correlations at short length scales, within the cluster, are treated explicitly with a quantum Monte Carlo (QMC) simulation, while those at longer length scale are treated at the mean field level. Due to the residual mean field character of our approximation, we expect our calculation to *overestimate the transition temperatures of both the DDW and DSC critical temperatures.*

Generally, we expect to see the the most pronounced mean-field behavior from the smallest cluster that can reflect the broken symmetry. A similar situation occurs in DMFA simulations of the antiferromagnetic phase of the Hubbard model, where Néel order is possible since the impurity spin and the mean-field host may have opposite spin orientations. Since non-local fluctuations are suppressed, the DMFA overestimates the Néel transition temperature. In the present case, the $N_c = 4$ (i.e. 2×2) is the smallest possible cluster allowing for d-wave pairing or a circulating current. Orbital antiferromagnetism is possible since the moment in the cluster and the host can have opposite orientations. Since fluctuations on longer length scales are suppressed, we would expect to overestimate both the d-wave superconducting and the d-density wave transition temperatures.

Formalism We present DCA calculations for the conventional 2D Hubbard model describing the dynamics of
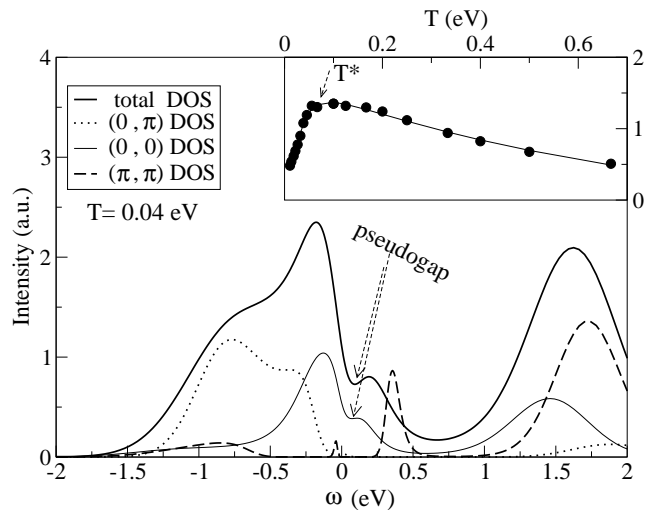

FIG. 1: The one particle total and K dependent DOS at $\delta = 0.05$ doping. Inset: The uniform magnetic susceptibility versus T. The maximum defines the pseudogap temperature T^*.

electrons on a square lattice. The model

$$H = -t \sum_{<i,j>,\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i\downarrow} n_{i\uparrow} \ , \qquad (1)$$

is characterized by a hopping integral t between nearest neighbor sites and a Coulomb repulsion U two electrons feel when residing on the same site. As the energy scale we set $t = 0.25$eV so that the band-width $W = 8t = 2$eV, and study the intermediate coupling regime $U = W$. We study the dynamics on short length-scales by setting the cluster size to $N_c = 4$. This cluster size is large enough to capture the qualitative low-energy physics of the cuprate superconductors [19, 20]. The corresponding phase diagram resembles the generic phase diagram of cuprates [20], displaying regions characterized by antiferromagnetism, d-wave superconductivity, Fermi liquid and pseudogap regimes, in qualitative agreement with experimental results.

In this paper we calculate the static (i.e. $\omega = 0$) susceptibilities which correspond to the circulating current (cc) operator,

$$W = i \sum_{k,\sigma} g(k) c_{k+Q,\sigma}^\dagger c_{k,\sigma} \ , \qquad (2)$$

and respectively to the d-wave pairing operator,

$$P = \sum_{k,\sigma} g(k) c_{k\downarrow} c_{-k\uparrow} \ , \qquad (3)$$

where $g(k) = \cos(k_x) - \cos(k_y)$ is the d-wave symmetry factor.

Results The pseudogap temperature, T^* is determined from the maximum in the uniform magnetic susceptibility (see the inset in Fig. 1) when accompanied by
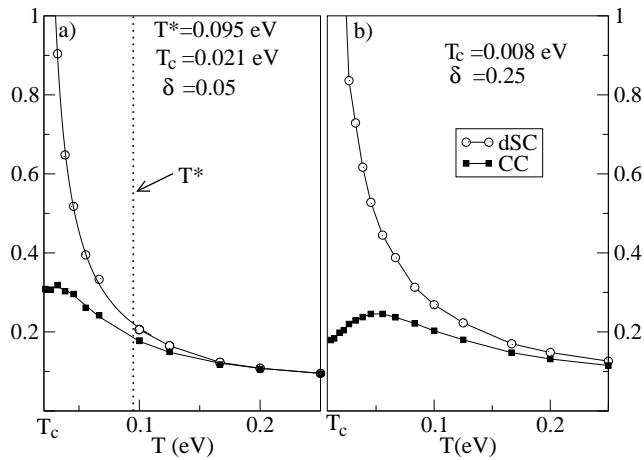
FIG. 2: The d-wave pairing (circles) and the circulating current (squares) susceptibilities versus temperature, at a) 5% and b) 25% doping. The dotted vertical line in a) is at the pseudogap temperature T^*.

a suppression of spectral weight in the DOS. We show this in Fig. 1 where the total and the K-dependent DOS, below T^*, at $\delta = 0.05$ doping is plotted. The DCA on a $N_c = 4$ cluster implies a coarse graining of the Brillouin Zone in four cells around $K = (0,0)$, $(0,\pi)$, $(\pi,0)$ and (π,π) and the K-dependent DOS corresponds to the average over all k belonging to a coarse-grained cell of the single particle spectra $A(k,\omega)$. This poor resolution in the reciprocal space allows to study only the gross features in the single-particle spectra. Despite this, it can be seen from Fig. 1 that the pseudogap in the total DOS is a result of the suppression of spectral weight in the cell at $(0,\pi)$. Therefore, we believe that our calculations capture well the experimentally observed features of the pseudogap.

However, our calculations show that these features are not a consequence of the DDW state. In Fig. 2-a we plot both the d-wave pairing susceptibility and the cc-susceptibility versus temperature, at $\delta = 0.05$ doping. The pairing susceptibility diverges at T_c, indicating a d-wave superconducting instability. The cc-susceptibility does not diverge, indicating the absence of a possible transition to the DDW state.

At large temperatures the d-wave pairing and the cc-susceptibilities are degenerate, and they both increase with decreasing temperature. In the pseudogap region (left side of dotted line) the d-wave pair field susceptibility is much larger than the cc-susceptibility. Close to T_c, the cc-susceptibility saturates and starts even decreasing with decreasing temperature. The fact that in the pseudogap region both d-wave and the cc-susceptibilities are enhanced show that fluctuations between these states are significant, as it was predicted by the $SU(2)$ theory [14].

In Fig. 2-b we show the d-wave and the cc-susceptibilities at $\delta = 0.25$ doping. No pseudogap [20]

is observed at this doping. We notice that, starting well above T_c, the cc-susceptibility decreases with decreasing temperature. This behavior is different from the one observed at small doping where the cc-susceptibility increases with decreasing T up to T_c. We therefore conclude that in the overdoped region the fluctuations between DSC and DDW above T_c are much less important.

Calculations (not shown here) with other values of the parameters (different values of U), or with the inclusion of next-nearest-neighbor hopping corresponding to both electron and hole doping, exhibit similar results. A divergent DDW susceptibility is never found. Our results are consistent with renormalization group studies [21] where no divergence of the cc-susceptibility is found, and with a mean-field treatment of an extended Hubbard model[22] where an additional correlated hopping term was necessary to stabilize the DDW state.

Conclusions We present a DCA calculation of the two-dimensional Hubbard model, focusing on the competition between DDW and DSC orders. We showed previously that the DCA calculation captures the generic features of the pseudogap region as seen in the photoemission and magnetic measurements. Nevertheless, as we show here, these properties are not a consequence of the existence of DDW state. The DCA should overestimate any DDW transition temperature but, despite this, we found no transition to such state.

We also found that both the cc-susceptibility and the d-wave pairing susceptibility are enhanced in the pseudogap region, indicating that the fluctuations between these states is significant. This is not true in the overdoped region, where we found that the cc-susceptibility is suppressed above T_c.

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